# Separable Structure of Many-Body Ground-State Wave Function

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**Abstract**

We have investigated a general structure of the ground-state wave function for the Schrödinger equation for $N$ identical interacting particles (bosons or fermions) confined in a harmonic anisotropic trap in the limit of large $N$. It is shown that the ground-state wave function can be written in a separable form. As an example of its applications, this form is used to obtain the ground-state wave function describing collective dynamics for $N$ trapped bosons interacting via contact forces.

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The structure of the ground-state wave function for a many-body system is very important for theoretical understanding of recently observed Bose-Einstein condensation (BEC) [1] (the theoretical aspects of the BEC are discussed in recent reviews [2]) and other many body problems. The Ginzburg-Pitaevskii-Gross (GPG) equation [3] is most widely used to describe the experimental results for the BEC. Recently, an alternative method of equivalent linear two-body (ELTB) equations for many body systems has been developed based on the variational principle [4,5]. In this paper, we consider $N$ identical particles (bosons or fermions) confined in a harmonic anisotropic trap. We show that in the case of large $N$ the ground-state wave function can be written in separable form as

$$\Psi(\vec{r}_1, \vec{r}_2, ...\vec{r}_N) = \phi(x, y, z) \cdot \chi(\Omega, \sigma), \tag{1}$$

where

$$x = \sqrt{\sum_{i=1}^{N} x_i^2}, \quad y = \sqrt{\sum_{i=1}^{N} y_i^2}, \quad z = \sqrt{\sum_{i=1}^{N} z_i^2}, \tag{2}$$

$\Omega$ is a set of (3N - 3) angular variables, and $\sigma$ is a set of spin variables.

We start from a generalization of the hyperspherical expansion of the wave function for the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i + \frac{1}{2}m\sum_{i=1}^{N}(\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) + \sum_{i<j} V_{int}(\mathbf{r}_i - \mathbf{r}_j) \tag{3}$$

in the form [4,6]

$$\Psi(\mathbf{r}_1, ...\mathbf{r}_N) = \sum_{[K]} \Phi_{[K]}(x, y, z) Y_{[K]}(\Omega_x^N, \Omega_y^N, \Omega_z^N, \sigma), \tag{4}$$

where $Y_{[K]}(\Omega_x^N, \Omega_y^N, \Omega_z^N, \sigma) = Y_{K_x,K_y,K_z}^{\nu_x,\nu_y,\nu_z}(\Omega_x^N, \Omega_y^N, \Omega_z^N, \sigma)$ is the combination of the hyperspherical harmonics, $Y_{K_x}^{\nu_x}(\Omega_x^N), Y_{K_y}^{\nu_y}(\Omega_y^N)$, and $Y_{K_z}^{\nu_z}(\Omega_z^N)$, with functions of spin variables $\sigma$, which is symmetric or antisymmetric with respect to

permutations of particles for bosons or fermions respectively. $[K]$ represents a set of numbers $[K_x, \nu_x, K_y, \nu_y, K_z, \nu_z]$.

The hyperspherical harmonics $Y^{\nu_x}_{K_x}(\Omega^N_x)$, $Y^{\nu_y}_{K_y}(\Omega^N_y)$, and $Y^{\nu_z}_{K_z}(\Omega^N_z)$ are eigenfunctions of the hyperspherical angular parts of the Laplace operators $\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2}$, $\sum_{i=1}^{N} \frac{\partial^2}{\partial y_i^2}$, and $\sum_{i=1}^{N} \frac{\partial^2}{\partial z_i^2}$, respectively.

The Laplace operators are defined by

$$\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} = \frac{1}{x^{N-1}} \frac{\partial}{\partial x}(x^{N-1} \frac{\partial}{\partial x}) + \frac{1}{x^2} \Delta_{\Omega^N_x},$$

$$\sum_{i=1}^{N} \frac{\partial^2}{\partial y_i^2} = \frac{1}{y^{N-1}} \frac{\partial}{\partial y}(y^{N-1} \frac{\partial}{\partial y}) + \frac{1}{y^2} \Delta_{\Omega^N_y}, \qquad (5)$$

and

$$\sum_{i=1}^{N} \frac{\partial^2}{\partial z_i^2} = \frac{1}{z^{N-1}} \frac{\partial}{\partial z}(z^{N-1} \frac{\partial}{\partial z}) + \frac{1}{z^2} \Delta_{\Omega^N_z}.$$

The hyperspherical angles $\theta^x_1, \theta^x_2, ...\theta^x_{N-1}, \theta^y_1, \theta^y_2, ...\theta^y_{N-1}, \theta^z_1, \theta^z_2, ...\theta^z_{N-1}$ can be chosen in such a way that the hyperspherical angular parts of the Laplace operators $\Delta_{\Omega^N_t}$ satisfy the recursion relation [7]

$$\Delta_{\Omega^N_u} = \frac{1}{\sin^{N-2}\theta^u_{N-1}} \frac{\partial}{\partial \theta^u_N}(\sin^{N-2}\theta^u_{N-1} \frac{\partial}{\partial \theta^u_{N-1}}) + \frac{1}{\sin^2 \theta^u_{N-1}} \Delta_{\Omega^{N-1}_u} \qquad (6)$$

with $u = x, y$, or $z$.

Functions $\Phi_{[K]}(x, y, z)$ satisfy equations

$$\sum_{[K']} h_{[K],[K']} \Phi_{[K']}(x, y, z) = E\Phi_{[K]}(x, y, z), \qquad (7)$$

where

$$h_{[K][K']} = \delta_{K_x K_x'}\delta_{K_y K_y'}\delta_{K_z K_z'}\delta_{\nu_x \nu_x'}\delta_{\nu_y \nu_y'}\delta_{\nu_z \nu_z'}[-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})$$

$$+\frac{m}{2}(\omega_x^2 x^2+\omega_y^2 y^2+\omega_z^2 z^2)+\frac{\hbar^2}{2m}(\frac{(N-1+2K_x)(N-3+2K_x)}{4x^2}$$

$$+\frac{(N-1+2K_y)(N-3+2K_y)}{4y^2}+\frac{(N-1+2K_z)(N-3+2K_z)}{4z^2}]$$

$$+V_{[K][K']}(x,y,z), \tag{8}$$

with

$$V_{[K][K']}(x,y,z) =< K_x,\nu_x,K_y,\nu_y,K_z,\nu_z \mid \sum_{i<j} V_{int}(\mathbf{r}_i - \mathbf{r}_j) \mid K_x',\nu_x',K_y',\nu_y',K_z',\nu_z' > . \tag{9}$$

We write $\Phi_{[K]}(x,y,z)$ in the form of a Laplace integral

$$\Phi_{[K]}(x,y,z) = \int f_{[K]}(\alpha_x,\alpha_y,\alpha_z)\phi_x(x,\alpha_x)\phi_y(y,\alpha_y)\phi_z(z,\alpha_z)d\alpha_x d\alpha_y d\alpha_z, \tag{10}$$

where

$$\phi_t(t,\alpha_t) = \sqrt{\frac{2}{\Gamma(N/2)}}(\frac{m\tilde{\omega}}{\alpha_t^2\hbar})^{N/4}\exp[-m\tilde{\omega}(\frac{t}{\alpha_t})^2/(2\hbar)]t^{(N-1)/2}, \tag{11}$$

and $\tilde{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$.

The Hill-Wheeler type equations [8,9] are obtained by requiring that energy of the system is stationary with respect to the functions $f_{[K]}(\alpha_x,\alpha_y,\alpha_z)$

$$\sum_{[K]}\int d\alpha_x d\alpha_y d\alpha_z f_{[K]}(\alpha_x,\alpha_y,\alpha_z)[H_{[K][K']}(\alpha_x\alpha_y\alpha_z,\alpha'_x\alpha'_y\alpha'_z)$$
$$-\delta_{[K][K']}S(\alpha_x\alpha_y\alpha_z,\alpha'_x\alpha'_y\alpha'_z)E]=0, \tag{12}$$

where

$$H_{[K][K']}(\alpha_x\alpha_y\alpha_z,\alpha'_x\alpha'_y\alpha'_z)=<\phi_x(x,\alpha_x)\phi_y(y,\alpha_y)\phi_z(z,\alpha_z)Y_{[K]}$$
$$\times\mid H\mid\phi_x(x,\alpha'_x)\phi_y(y,\alpha'_y)\phi_z(z,\alpha'_z)Y_{[K']}>, \tag{13}$$

and

$$S(\alpha_x\alpha_y\alpha_z,\alpha'_x\alpha'_y\alpha'_z)=<\phi_x(x,\alpha_x)\phi_y(y,\alpha_y)\phi_z(z,\alpha_z)\mid\phi_x(x,\alpha'_x)\phi_y(y,\alpha'_y)\phi_z(z,\alpha'_z)>. \tag{14}$$

In order to solve the Hill-Wheeler type equations (12), we assume that the integral in Eq. (10) can be replaced by sum

$$\Phi_{[K]}(x,y,z)=\sum_{i,j,k=1}^{\infty}c_{ijk}^{[K]}\phi_x(x,\alpha_x^i)\phi_y(y,\alpha_y^j)\phi_z(z,\alpha_z^k), \tag{15}$$

where $c_{ijk}^{[K]}$ are solutions of the following equations

$$\sum_{\substack{i',j',k'\\ [K']}}[H_{[K][K']}(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})-\delta_{[K][K']}S(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})E]c_{i'j'k'}^{[K']}=0. \tag{16}$$

For the case of large $N$, the overlap, Eq. (14),

$$S(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})=[\frac{8\alpha_x^i\alpha_x^{i'}\alpha_y^j\alpha_y^{j'}\alpha_z^k\alpha_z^{k'}}{((\alpha_x^i)^2+(\alpha_x^{i'})^2)((\alpha_y^j)^2+(\alpha_y^{j'})^2)((\alpha_z^k)^2+(\alpha_z^{k'})^2)}]^{N/2} \tag{17}$$

reduces to the Kronecker deltas

$$S(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})=\delta_{ii'}\delta_{jj'}\delta_{kk'} \tag{18}$$

Since the ratio

$$H_{[K][K']}(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})/S(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})$$

is a much more slowly varying function of $\alpha$ compared to $S(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha^{j'}y\alpha_z^{k'})$ in almost all cases [10], we have for the case of large $N$

$$H_{[K][K']}(\alpha_x^i\alpha_y^j\alpha_z^k,\alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})=\tilde{H}_{[K][K']}(\tilde{\alpha_x},\tilde{\alpha_y},\tilde{\alpha_z})\delta_{ii'}\delta_{jj'}\delta_{kk'}, \tag{19}$$

(see Appendix for the case of $N$ identical particles interacting via contact repulsive force).

Substitution of Eq. (19) into Eq. (16) gives

$$\Phi_{[K]}(x,y,z)=\tilde{c}_{[K]}\phi_x(x,\tilde{\alpha_x})\phi_y(y,\tilde{\alpha_y})\phi_z(z,\tilde{\alpha_z}), \tag{20}$$

where $\tilde{c}_{[K]}$ are solutions of the following equations

$$\sum_{[K']}[\tilde{H}_{[K][K']}(\tilde{\alpha_x},\tilde{\alpha_y},\tilde{\alpha_z})-\delta_{[K][K']}E]\tilde{c}_{[K']}, \tag{21}$$

and parameters $\tilde{\alpha_x},\tilde{\alpha_y}$, and $\tilde{\alpha_z}$ are solutions of

$$\frac{\partial E}{\partial\tilde{\alpha_x}}=\frac{\partial E}{\partial\tilde{\alpha_y}}=\frac{\partial E}{\partial\tilde{\alpha_z}}=0.$$

Substitution of Eq. (20) into Eq. (4) yields $\Psi(\vec{r}_1,\vec{r}_2,...\vec{r}_N)$ given by Eq. (1) with

$$\phi(x,y,z)=\phi_x(x,\tilde{\alpha_x})\phi_y(y,\tilde{\alpha_y})\phi_z(z,\tilde{\alpha_z}),$$

and

$$\chi(\Omega,\sigma)=\sum_{[K]}\tilde{c}^{[K]}Y_{[K]}(\Omega_x^N,\Omega_y^N,\Omega_z^N,\sigma).$$

We now consider $N$ identical particles confined in an anisotropic harmonic trap and interacting via contact force

$$V_{int}(\vec{r}_i-\vec{r}_j)=\frac{4\pi\hbar^2 a}{m}\delta(\vec{r}_i-\vec{r}_j), \tag{23}$$

with positive scattering length $a>0$. Using factorization (1) we have

$$[-\tfrac{\hbar^2}{2m}(\tfrac{\partial^2}{\partial x^2}+\tfrac{\partial^2}{\partial y^2}+\tfrac{\partial^2}{\partial z^2})+\tfrac{m}{2}(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2)-\tfrac{\hbar^2}{2m}(\tfrac{c_x}{x^2}+\tfrac{c_y}{y^2}+\tfrac{c_z}{z^2})$$

$$+\tfrac{\hbar^2}{2m}\tfrac{(N-1)(N-3)}{4}(\tfrac{1}{x^2}+\tfrac{1}{y^2}+\tfrac{1}{z^2})+\tfrac{c}{xyz}]\phi(x,y,z)=E\phi(x,y,z), \tag{24}$$

where $c_t=<\chi\mid\Delta_{\Omega_t^N}\mid\chi>/<\chi\mid\chi>$ with $t=(x,y,z)$ and

$$c=\frac{a\hbar^2N(N-1)}{\sqrt{2\pi}m}(\frac{\Gamma(N/2)}{\Gamma((N-1)/2)})^3\tilde{c}.$$

In the large $N$ limit, parameters $c_x,c_y,c_z$, and $\tilde{c}$ are expected to be slowly varying functions of $N$. For $N$ identical bosonic atoms with large $N$, an essentially exact expression for the ground state energy can be obtained by neglecting the kinetic energy term in the GPG equation [2,3] (this is called "Thomas-Fermi approximation" [11]). From comparison of the ground state solution of Eq. (24) with the Thomas-Fermi approximation [11], we can fix unknown parameters and find the ground-state solution of Eq. (24) as

$$\phi(x,y,z)=\psi_x(x)\psi_y(y)\psi_z(z), \tag{25}$$

$$E=\frac{5N\hbar\tilde{\omega}}{4}\tilde{n}^{2/5}, \tag{26}$$

with

$$\begin{aligned}\psi_x(x) &= Ax^{(N-1)/2}\exp[-m\tilde{\omega}(x/\alpha)^2/(2\hbar)],\\ \psi_y(y) &= Ay^{(N-1)/2}\exp[-m\tilde{\omega}(y/\beta)^2/(2\hbar)],\\ \psi_z(z) &= Az^{(N-1)/2}\exp[-m\tilde{\omega}(z/\gamma)^2/(2\hbar)],\end{aligned} \tag{27}$$

where $A = \sqrt{2/\Gamma(N/2)}(m\tilde{\omega}/(\alpha^2\hbar))^{N/4}$, $\alpha = \tilde{n}^{1/5}\tilde{\omega}/\omega_x$, $\beta = \tilde{n}^{1/5}\tilde{\omega}/\omega_y$, $\gamma = \tilde{n}^{1/5}\tilde{\omega}/\omega_z$, $\tilde{\omega} = (\omega_x\omega_y\omega_z)^{1/3}, \tilde{n} = n\tilde{c}, n = 2\sqrt{\tilde{\omega}m/(2\pi\hbar)}Na$ and

$$\tilde{c} = (\frac{4}{7})^{5/2}\frac{15}{8}\sqrt{\pi} \approx 0.82. \tag{28}$$

Eqs. (25-28) give the exact ground-state solution of Eq. (24) for large $N$. Thus we have found an analytical solution for the ground-state wave function describing collective dynamics in variables (x,y,z) in the large $N$ limit.

We note that the slope of the Thomas-Fermi wave function becomes infinity at the surface, leading to logarithmic singularity in the kinetic energy. Hence it is necessary to modify the Thomas-Fermi wave function near the surface [12-14]. In contrast, we do not have such problems for our solution, Eq. (25-28).

It is also interesting to compare our results with the ELTB method [4,5]. For this situation (contact force, Eq. (23) and large N limit), the ELTB method corresponds to $\tilde{c}^{2/5} = 1$. It shows that the ELTB method is a very good approximation with relative error of about 8% for parameter $\tilde{c}^{2/5}$.

In summary, we have investigated the general structure of the ground-state solution of the Schrödinger equation for $N$ identical interacting particles (bosons or fermions) confined in a harmonic anisotropic trap in the large $N$ limit. The main results and conclusions are as follows

(i) It has been shown that in the case of large $N$ the ground-state wave function can be written in separable form, Eq. (1).

(ii) Using this form, we have found an analytical solution for the ground-state wave function, Eqs. (25-29), describing collective dynamics in collective variables (x,y,z) for $N$ trapped bosons interacting via contact repulsive forces.

(iii) Our results can be used for checking various approximations (both existing and future) made for the Schrödinger equation describing $N$ identical interacting particles (bosons or fermions) confined in a harmonic anisotropic trap.

## Appendix

To prove Eq. (19) we consider the contact potential case

$$V_{int}(\mathbf{r}_i - \mathbf{r}_j, \sigma) = \delta(\mathbf{r}_i - \mathbf{r}_j)\eta(\sigma), \qquad (A.1)$$

where $\eta$ depends on spin variables. Using Eq. (A.1) we can rewrite Eq. (9) as

$$V_{[K][K']}(x, y, z) = \gamma_{[K][K']}\frac{N(N-1)}{xyz}, \qquad (A.2)$$

where $\gamma_{[K][K']}$ does not depend on $x, y, z$.

Substitution of Eq. (A.2) into Eq. (13) gives

$$H_{[K][K']}(\alpha_x^i\alpha_y^j\alpha_z^k, \alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})/(\hbar\tilde{\omega}N) = (1/2)S(\alpha_x^i\alpha_y^j\alpha_z^k, \alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})$$

$$\times[\delta_{[K][K']}(\frac{1+(\alpha_x^i)^2(\alpha_x^{i'})^2\beta_x^2}{(\alpha_x^i)^2+(\alpha_x^{i'})^2} + \frac{1+(\alpha_y^j)^2(\alpha_y^{j'})^2\beta_y^2}{(\alpha_y^j)^2+(\alpha_y^{j'})^2} + \frac{1+(\alpha_z^k)^2(\alpha_z^{k'})^2\beta_z^2}{(\alpha_z^k)^2+(\alpha_z^{k'})^2})$$

$$+\frac{\sqrt{((\alpha_x^i)^2+(\alpha_x^{i'})^2)((\alpha_y^j)^2+(\alpha_y^{j'})^2)((\alpha_z^k)^2+(\alpha_z^{k'})^2)}}{\alpha_x^i\alpha_x^{i'}\alpha_y^j\alpha_y^{j'}\alpha_z^k\alpha_z^{k'}}(\frac{\Gamma((N-1)/2)}{\Gamma(N/2)})^3$$

$$\times(\frac{m\tilde{\omega}}{\hbar})^{3/2}\frac{N-1}{\sqrt{8}}\gamma_{[K][K']}], \qquad (A.3)$$

where $\beta_t = \omega_t/\tilde{\omega}$ for $t = x, y$, or $z$.

For large $N$, $S(\alpha_x^i\alpha_y^j\alpha_z^k, \alpha_x^{i'}\alpha_y^{j'}\alpha_z^{k'})$, Eq. (14), reduces to the Kronecker deltas $\delta_{ii'}\delta_{jj'}\delta_{kk'}$, and hence from Eq. (A.3) we obtain Eq. (19).

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